

# State determination: an iterative algorithm.

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An iterative algorithm for state determination is presented that uses as physical input the probability distributions for the eigenvalues of two or more observables in an unknown state  $\Phi$ . Starting from an arbitrary state  $\Psi_0$ , a succession of states  $\Psi_n$  is obtained that converges to  $\Phi$  or to a Pauli partner. This algorithm for state reconstruction is efficient and robust as is seen in the numerical tests presented and is a useful tool not only for state determination but also for the study of Pauli partners. Its main ingredient is the Physical Imposition Operator that changes any state to have the same physical properties, with respect to an observable, of another state.

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## I. INTRODUCTION

At an early stage in the development of quantum mechanics, W. Pauli [1] raised the question whether the knowledge of the probability density functions for the position and momentum of a particle were sufficient in order to determine its state. That is, can we determine a unique  $\psi(x)$  if we are given  $\rho(x) = |\psi(x)|^2$  and  $\pi(p) = |\phi(p)|^2$ , where  $\phi(p)$  is the Fourier transform of  $\psi(x)$ ? Since position and momentum are the unique independent observables of the system, it was, erroneously, guessed that this Pauli problem could have an affirmative answer. This was erroneous because there may be different quantum correlations between position and momentum that are not reflected in the distributions of position and momentum individually. Indeed, many examples of Pauli partners, that is, different states  $\psi_1 \neq \psi_2$  with identical probability distributions  $\rho$  and  $\pi$ , were found. A review of these issues, with references to the original papers, and the treatment of the problem of state reconstruction for finite and infinite dimension of the Hilbert space, can be found in refs. [2, 3]. The general problem of the determination of a quantum state from laboratory measurements turned out to be a difficult one. In this work the “laboratory measurement” means the complete measurement of an observable, that is, the determination of the probability distribution  $\varrho(a_k)$  of the eigenvalues  $a_k$  of the operator  $A$  associated with the observable. Given a state  $\Phi$ , the

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probability distribution (assuming non-degeneracy) is given by  $\varrho(a_k) = |\langle \varphi_k, \Phi \rangle|^2$  where  $\varphi_k$  are the eigenvectors of the operator. The state is not directly observable; what can be measured, are the probability distributions of the eigenvalues of the observables and we want to be able to determine the state  $\Phi$  of the system using these distributions. Besides the academic interest of quantum state reconstruction based on measurements of probability distributions, the issue has gained actuality in the last decade in the possible practical applications of quantum information theory [4].

In order to state clearly the problem, let us consider a system described in an  $N$  dimensional Hilbert space. The determination of the state requires the determination of  $2N - 2$  real numbers and a complete measurement of an observable provides  $N - 1$  equations. With the measurement of two observables (like position and momentum in the Pauli problem) we have the same number of equations as unknowns. However the equations available are not linear and the system of equations will not have, in general, a unique solution. In many practical cases, a minimal additional information (like the sign of an expectation value) is sufficient to determine the state. In this work we will not search the minimal extra information required, but instead, we will add a complete measurement of a third observable. One may think that this massive addition of information will make the system over-determined and that with three complete measurements we should always be able to find a unique state. This is wrong; there are pathological cases where the complete measurement of  $N$  observables, that is  $N(N - 1)$  equations, is *not sufficient* for the determination of a *unique* set of  $2(N - 1)$  numbers! In the other extreme, if the state happens to be equal to one of the eigenvectors of the observable measured, then, of course, just one complete measurement is sufficient to fix the state. From these two cases we conclude that the choice of the observables to be measured is crucial for the determination of the state; an observable with a probability distribution peaked provides much more information than an observable with uniform distribution. A pair of observables may provide redundant information and we expect that it is convenient to use observables as different as possible; this happens when their eigenvectors build two unbiased bases as is the case, for example, with position and momentum (two bases  $\{\varphi_k\}$  and  $\{\phi_r\}$  are unbiased when  $|\langle \varphi_k, \phi_r \rangle| = 1/\sqrt{N} \forall k, r$ , that is, every element of one basis has equal “projection” on all elements of the other basis). For this reason, unbiased bases have been intensively studied in the problem of state determination and also in quantum information theory [5, 6, 7]. The number of mutually unbiased bases that one can define in an  $N$  dimensional Hilbert space is not known in general although it can be proved that if  $N$  is equal to a power of a prime number, then there are  $N + 1$  unbiased bases. *Unbiased observables*, those represented by operators whose eigenvectors build unbiased bases, provide independent information; there are however pathological cases where the measurement of several unbiased observables is useless to determine a unique state: assume for instance that the state belongs to a basis that is unbiased to several other mutually unbiased bases associated with the measured observables. In this case all the probability distributions are uniform and the state can not be uniquely determined because there are at least  $N$  different states (corresponding to the  $N$  elements of the basis to which the state belongs) all generating

uniform distributions for the observables. If  $N$  is a power of a prime number we could have up to  $N$  observables with uniform distributions for  $N$  different states. This is the pathological case mentioned before: if there are  $N + 1$  mutually unbiased bases and we have  $M$  unbiased observables with uniform distributions then we have  $N(N + 1 - M)$  Pauli partners, that is, different states having the same distributions.

If we make complete measurements of two or more observables we should be able to determine the state but it will not always be unique because there may be several different states having the same distributions for the measured observables. If we measure three observables, the mathematical problem would be to solve a set of  $3N - 3$  nonlinear equations to determine  $2N - 2$  numbers. One could blindly apply some numerical method to find the solution. Instead of this, we present in this work an iterative method that is physically appealing because it involves the imposition of physical data to Hilbert space elements that are approaching the solution. Another advantage of this algorithm is that it does not involve the solution of a system of equations and therefore when we change the number of observables measured or the dimension of the Hilbert space, we only have to make a trivial change in the algorithm. We will test the algorithm numerically by assuming an arbitrary state and two, three or four arbitrary observables, with them we generate the data corresponding to the distributions of the observables in the chosen state, and then we run the algorithm and we see how efficiently it returns the chosen state.

## II. A METRIC FOR STATES

In order to study the convergence of an iterative algorithm for the determination of a state, we will need a concept of *distance* that can tell us how close we are from the wanted solution. This criteria of approach can be applied in the space of states or in the space of probability distributions. In the first case we want to know how close a particular state is from the state searched, that is, we need a *metric in the space of states*. In the other case a particular state generates probability distributions for some observables and we want to know how close these distribution are from the corresponding distributions generated by the state searched. In this second case we need a *metric in the space of distributions*. The relation between these two distances in two different spaces has been studied for several choices of distances [8]. However the application of some of these “distances” that do not satisfy the mathematical requirements of a “metric” (positivity, symmetry and triangular inequality) in an iterative algorithm is questionable. In this work we use a metric in the Hilbert space of states in order to study the convergence of the algorithm but we also compare the final probability distributions with the corresponding distributions used as physical input for the algorithm because, as was explained before, there are cases of different states generating the same probability distributions. The usual Hilbert space metric induced by the norm, itself induced by the internal product,

$$\delta(\Psi, \Phi) = \|\Psi - \Phi\| = \sqrt{\langle \Psi - \Phi, \Psi - \Phi \rangle} \quad (1)$$

is not an appropriate metric for states because the states are not represented by Hilbert space elements but by *rays*, that are sets of Hilbert space elements with an arbitrary phase. That is, a state is given by

$$R_\Psi = \{e^{i\alpha}\Psi \mid \forall \alpha, \|\Psi\| = 1\} \quad (2)$$

The Hilbert space element  $\Psi$  is a *representant* of the ray and it is common practice in quantum mechanics to say that the state is given by  $\Psi$ . However when we deal with distance between states we can not take the induced metric mentioned before, because this metric for two Hilbert space elements,  $e^{i\alpha}\phi$  and  $e^{i\beta}\phi$ , belonging to the *same* ray, that is, belonging to the same state, does not vanish. A correct concept of distance between states is given by the distance between sets

$$d(R_\Psi, R_\Phi) = \min_{\alpha, \beta} \delta(e^{i\alpha}\Psi, e^{i\beta}\Phi) . \quad (3)$$

The minimization can be performed in general and we obtain

$$d(R_\Psi, R_\Phi) = \sqrt{2}\sqrt{1 - |\langle\Psi, \Phi\rangle|} . \quad (4)$$

We compare this result with  $\delta(\Psi, \Phi) = \sqrt{2}\sqrt{1 - \Re\langle\Psi, \Phi\rangle}$  and we conclude that  $d(R_\Psi, R_\Phi) \leq \delta(\Psi, \Phi)$  and therefore every sequence converging in the induced metric is also convergent in the ray metric used here.

In order to have a rigorous concept of convergence we must check that the distance between states given above in Eqs.(3,4) is really a metric (in general, for arbitrary sets, the distance between sets is not always a metric since one can easily find examples that violate the triangle inequality). The requirement of symmetry and positivity are trivially satisfied but to prove that this distance satisfies the triangle inequality is not trivial. However we can be sure that the distance between states is a metric because, in this particular case where the sets are rays, the distance between rays has the same value as the Hausdorff distance and one can prove that the Hausdorff distance is a metric [9]. The Hausdorff distance between two sets  $X$  and  $Y$  is defined by

$$d^H(X, Y) = \max \left\{ \sup_{x \in X} d(x, Y), \sup_{y \in Y} d(y, X) \right\} . \quad (5)$$

As a final comment in this section, notice that the square root in Eq.(4) is a nuisance but it can not be avoided because expressions like  $1 - |\langle\Psi, \Phi\rangle|$  or  $1 - |\langle\Psi, \Phi\rangle|^2$  are *not* metrics. In order to simplify the notation, in what follows, we will denote the distance between rays  $d(R_\Psi, R_\Phi)$  simply by  $d(\Psi, \Phi)$ .

### III. THE PHYSICAL IMPOSITION OPERATOR

A state, or a Hilbert space element, contains encoded information about all the observables of the system. Given a state  $\Phi$ , the probability distribution for an observable  $A$  is given by  $\varrho(a_k) = |\langle\varphi_k, \Phi\rangle|^2$  where  $\varphi_k$  are the eigenvectors of the operator  $A$  associated with the observable

corresponding to the eigenvalue  $a_k$ . Given any state  $\Psi$ , we can impose to this state the same distribution that the observable  $A$  has in the state  $\Phi$  by means of an operator, the *Physical Imposition Operator*,  $T_{A\Phi}$  that involves the expansion of  $\Psi$  in the basis  $\{\varphi_k\}$  of  $A$  and a change in the modulus of the expansion coefficients. That is

$$T_{A\Phi}\Psi = \sum_k |\langle\varphi_k, \Phi\rangle| \frac{\langle\varphi_k, \Psi\rangle}{|\langle\varphi_k, \Psi\rangle|} \varphi_k . \quad (6)$$

If  $\langle\varphi_k, \Psi\rangle = 0$  we assume zero phase, that is  $\langle\varphi_k, \Psi\rangle/|\langle\varphi_k, \Psi\rangle| = 1$ . The moduli of the expansion coefficients are changed in order to impose the distribution of the observable  $A$  in the state  $\Phi$  but the phases are retained and therefore some information of the original state  $\Psi$  is kept in the phases. Although the numerical treatment of this operator is straightforward, its mathematical features are not simple. The operator is idempotent  $T^2 = T$ , it has no inverse and it is not linear but  $T(c\Psi) = (c/|c|)T(\Psi)$ . Furthermore the operator is bounded because  $\|T\Psi\| = \|\Phi\| = 1$ . The fix points of this nonlinear application is the set of states that have the same distribution for the observable  $A$  as the state  $\Phi$ .

We will use this operator in order to develop an iterative algorithm for the determination of a state  $\Phi$  using as physical input the distribution of several observables in this state. It is therefore interesting to study whether this operator, applied to an arbitrary Hilbert space element  $\Psi$ , brings us closer to the state  $\Phi$  or not. For this we can compare the distance  $d(\Psi, \Phi)$  with the distance  $d(T_{A\Phi}\Psi, \Phi)$  for some given observable  $A$  and some state  $\Phi$ . Let us then define an observable  $A$  by choosing its eigenvectors  $\{\varphi_k\}$  (a basis) in a three dimensional Hilbert space,  $N = 3$ , and in this space let us take an arbitrary state  $\Phi$ . Now we consider a large number (8000) of randomly chosen states  $\Psi$  and draw a scatter plot of the distances of this state to  $\Phi$  before and after applying the imposition operator  $T_{A,\Phi}$ . In Figure 1 we see that there are more points below the diagonal, showing cases where the imposition operator brings us closer to the state but there are also many cases where the operator take us farther away from the searched state. We will later see that this has the consequence that the iterative algorithm will not converge for every starting point.

The imposition operator will shift the state  $\Psi$  some distance  $d(T_{A\Phi}\Psi, \Psi)$  that is smaller than the total distance to the state  $d(\Psi, \Phi)$ . That is, there is no “overshoot” that could undermine the convergence of the iterative algorithm. In order to prove this, consider the internal product

$$\begin{aligned} \langle T_{A\Phi}\Psi, \Psi \rangle &= \left\langle \sum_k |\langle\varphi_k, \Phi\rangle| \frac{\langle\varphi_k, \Psi\rangle}{|\langle\varphi_k, \Psi\rangle|} \varphi_k, \sum_r \langle\varphi_r, \Psi\rangle \varphi_r \right\rangle \\ &= \sum_k |\langle\varphi_k, \Phi\rangle| |\langle\varphi_k, \Psi\rangle| = \sum_k |\langle\Phi, \varphi_k\rangle \langle\varphi_k, \Psi\rangle| \\ &\geq \left| \sum_k \langle\Phi, \varphi_k\rangle \langle\varphi_k, \Psi\rangle \right| = |\langle\Phi, \Psi\rangle| . \end{aligned} \quad (7)$$

Now, using this inequality in the definition of distance in Eq.(4) we get

$$d(T_{A\Phi}\Psi, \Psi) \leq d(\Psi, \Phi) . \quad (8)$$

We can notice in Figure 1 that there is a bound for the distance  $d(T_{A\Phi}\Psi, \Phi)$  at some value smaller than the absolute bound for the distance  $\sqrt{2}$ . We will see that this bound appears when the state  $\Phi$  is chosen close to one of the eigenvectors of  $A$ . From the definition of the distance and of the imposition operator it follows easily that the distance of  $T_{A\Phi}\Psi$  to any element of  $\{\varphi_k\}$  is the same as the distance of  $\Phi$  to the same element. That is,

$$d(T_{A\Phi}\Psi, \varphi_k) = d(\Phi, \varphi_k) \quad \forall k, \quad (9)$$

so that  $T_{A\Phi}\Psi$  is something like a “mirror image” of  $\Phi$  reflected on  $\{\varphi_k\}$ . We can now use this in order to derive the bound mentioned. Consider the triangle inequality  $d(T_{A\Phi}\Psi, \Phi) \leq d(T_{A\Phi}\Psi, \varphi_k) + d(\Phi, \varphi_k)$ . Using Eq.(9), we get  $d(T_{A\Phi}\Psi, \Phi) \leq 2d(\Phi, \varphi_k)$ . Now we specialize this inequality for the value of  $k$  that minimizes the right hand side, that is, the value of  $k$  that maximizes  $|\langle \varphi_k, \Phi \rangle|$  or equivalently  $\sqrt{\rho(a_k)}$ . Then we have

$$d(T_{A\Phi}\Psi, \Phi) \leq 2 \min_k d(\Phi, \varphi_k) = 2\sqrt{2} \sqrt{1 - \max_k \sqrt{\rho(a_k)}}. \quad (10)$$

If the state  $\Phi$  is close enough to one of the eigenvectors of  $A$ , the corresponding maximum value of the distribution can be larger than 9/16 and the bound derived is smaller than the absolute bound  $\sqrt{2}$ . With increasing dimension  $N$  of the Hilbert space, the probability that a randomly chosen state is close to one of the basis elements decreases.

The physical imposition operator modifies the moduli of the expansion coefficients but leaves the phases unchanged. The reason for choosing this definition is that the moduli of the coefficients are measured in an experimental determination of the probability distribution of the eigenvalues of an observable and therefore this operator provides a way to impose physical properties to a state. It is unfortunate that the phases of the expansion coefficients are not directly accessible in an experiment because we could use the knowledge of the phases in a much more efficient algorithm. In a sense that will become clear later, the phases have more information about the state than the moduli. In order to clarify this let us define a *Phase Imposition Operator*  $P_{A\Phi}$  that leaves the moduli of the expansion coefficients unchanged but imposes the phases of the state  $\Phi$ . That is

$$P_{A\Phi}\Psi = \sum_k |\langle \varphi_k, \Psi \rangle| \frac{\langle \varphi_k, \Phi \rangle}{|\langle \varphi_k, \Phi \rangle|} \varphi_k. \quad (11)$$

The same as was done before, we study how efficiently this operator approaches to the state  $\Phi$ . In Figure 2 we see the corresponding scatter plot for the same operator and states of those in Fig.1, that shows that in *all* cases the application of this operator brings us closer to the wanted state. One can indeed prove that  $d(P_{A\Phi}\Psi, \Phi) \leq d(\Psi, \Phi)$  considering the internal product

$$\begin{aligned} \langle P_{A\Phi}\Psi, \Phi \rangle &= \left\langle \sum_k |\langle \varphi_k, \Psi \rangle| \frac{\langle \varphi_k, \Phi \rangle}{|\langle \varphi_k, \Phi \rangle|} \varphi_k, \sum_r \langle \varphi_r, \Phi \rangle \varphi_r \right\rangle \\ &= \sum_k |\langle \varphi_k, \Psi \rangle| |\langle \varphi_k, \Phi \rangle| = \sum_k |\langle \Psi, \varphi_k \rangle \langle \varphi_k, \Phi \rangle| \\ &\geq \left| \sum_k \langle \Psi, \varphi_k \rangle \langle \varphi_k, \Phi \rangle \right| = |\langle \Psi, \Phi \rangle|. \end{aligned} \quad (12)$$

Using this inequality in the definition of distance in Eq.(4) we get the inequality above. As said before, if we had physical information about the phases of the expansion coefficients, we could devise a very efficient algorithm. Unfortunately we don't have experimental access to the phases and this, in principle interesting, operator will no be further studied here.

#### IV. THE ALGORITHM FOR STATE DETERMINATION

In this section we will investigate an algorithm for state determination that uses as physical input the knowledge provided by the complete measurement of several observables. These measurements provide the probability distributions for the eigenvalues in the unknown state  $\Phi$ . In other words, we assume that we know the physical imposition operators  $T_{A\Phi}, T_{B\Phi}, T_{C\Phi} \dots$  for several observables. The algorithm basically consists in the iterative application of the physical imposition operators to some arbitrary initial state  $\Psi_0$  randomly chosen. Applying the operator  $T_{A\Phi}$  to the initial state  $\Psi_0$ , we will get closer to  $\Phi$  (although not always) but a second application of the operator is useless because  $T_{A\Phi}$  is idempotent. Then we use another operator for a closer approach, say  $T_{B\Phi}$ , and another one afterwards, until all physical information is used; then we start again with  $T_{A\Phi}$ . That is, we calculate the iterations  $\Psi_1, \Psi_2, \Psi_3 \dots$  given by  $\Psi_n = (\dots T_{B\Phi} T_{A\Phi})^n \Psi_0$  and the convergence  $\Psi_n \rightarrow \Phi$  is checked comparing the physical input, that is, the distributions associated with the observables  $A, B, C, \dots$ , with the corresponding distributions generated in the state  $\Psi_n$ .

In order to check the efficiency of the algorithm numerically, we choose a state  $\Phi$  at random and with it we generate the distributions corresponding to some observables that we use as input in the algorithm. Calculating the distance  $d(\Psi_n, \Phi)$  we study how efficiently the algorithm returns the initial state  $\Phi$ . There are cases where the algorithm converges to a state  $\Phi'$  different from  $\Phi$  but having the same physical distributions, that is, to a Pauli partner of  $\Phi$ . An interesting feature of the algorithm is that we can span the whole Hilbert space by choosing the starting states  $\Psi_0$  randomly and the algorithm delivers many, if not all, Pauli partners. We can not be sure that all Pauli partners are found because some of them could correspond to a starting state  $\Psi_0$  belonging to a set of null measure that will not be necessarily "touched" in a random sampling of the Hilbert space. This seems to be quite unlikely but it can not be excluded. In this way, the algorithm presented is not only a numerical tool for state determination but is also a useful tool for the theoretical investigation of the appearance of Pauli partners. An example of this is presented below.

The algorithm is very efficient; however there are some starting states  $\Psi_0$  where the algorithm fails to converge. It was not surprising to find these failures because, as was suggested in Fig. 1, the physical imposition operator sometimes take us farther away from the wanted state. We are informed of this failure because the distributions used as input are not approached in each iteration. In the case of a failure, we can simply restart the algorithm with a different initial state  $\Psi_0$  or restart with another initial state orthogonal to the one that failed. In this last case

the probability of a repeated failure is much reduced and therefore it is a convenient choice. The appearance of a failure depends strongly on the choice of observables used to determine the state. If we use three unbiased observables we very rarely found a failure, in less than 1% of the cases, but if we use three random observables (see below) 40% of the randomly chosen starting states  $\Psi_0$  fail but only 10% of these fail again if we restart with an orthogonal state. In the case of four angular momentum observables in four arbitrary directions we had to restart the algorithm in some 10% of the cases. The appearance of failures also depends on the shape of the distributions: when one of the distributions is peaked, that is, the maximum value of the distribution  $\rho(a_k)$  has a large value for some  $k$ , the application of the corresponding imposition operator bring us close to the wanted state as can be seen in Eq.(10), and Figure 1 shows that then the algorithm has better convergence and no failures are found. This has been confirmed in the numerical tests.

The convergence to the state  $\Phi$ , or to a Pauli partner, was tested numerically in several Hilbert space dimensions and for different choice of observables. These choices were random in some cases, that is, their associated orthonormal bases are randomly chosen, and in other cases we used physically relevant observables like angular momentum or position and momentum. Position and momentum observables are usually represented by unbound operators in infinite dimensional Hilbert spaces; however there are also realizations of these observables in finite dimensions, for instance in a cyclic lattice, where they are represented by unbiased operators [10, 11]. In general the operators  $T_{A\Phi}$ ,  $T_{B\Phi}$ ,  $\dots$  do not commute and the iteration of  $(\dots T_{B\Phi} T_{A\Phi})^n$  and  $(\dots T_{A\Phi} T_{B\Phi})^n$  are not necessarily equal. The algorithm was tested with several different choices in the ordering of the noncommuting physical imposition operators and also with random ordering and it turned out that the convergence of the algorithm is not much affected by the different orderings. The algorithm is robust under the noncommutativity of the observables.

The physical imposition operator  $T_{A\Phi}$  is idempotent so it is useless to apply it more than once (successively) in an attempt to approach the state  $\Phi$ . Clearly, the complete measurement of just one observable is not sufficient to determine the state, except in the trivial case when the state happens to be equal to one of the eigenvector of the operator. Therefore we consider the information provided by *two* observables  $A$  and  $B$  (for two unbiased observables, like  $X$  and  $P$ , this is precisely the Pauli problem). We studied then the convergence of  $\Psi_n = (T_{B\Phi} T_{A\Phi})^n \Psi_0$  towards  $\Phi$  or to a Pauli partner, for an arbitrary  $\Psi_0$ . In a three dimensional Hilbert space,  $N = 3$ , we applied the algorithm in several cases: for  $A$  and  $B$  random, unbiased (that is, of the type  $X$  and  $P$ ) and also for angular momentum operators  $J_x, J_y$ . As was expected, in all these cases the algorithm returned several Pauli partners. Choosing the starting state  $\Psi_0$  randomly (uniform distributed in the Hilbert space) we found that all Pauli partners found are accessed with similar frequency. As was mentioned before, we can not be sure that the algorithm will deliver *all* partners, however we may be confident that this may be so because in one particular case, where we can calculate exactly the number of partners, the algorithm returns them all. The particular case is the, so called, pathological case where we have uniform distributions for  $M$  observables that correspond



to  $N(N + 1 - M)$  partners. For several combinations of  $N$  and  $M$ , the algorithm delivered all partners.

Next we studied the case with *tree* operators providing physical information to determine the state (also with Hilbert space dimension  $N = 3$ ). We studied then the iteration  $\Psi_n = (T_{A\Phi}T_{B\Phi}T_{C\Phi})^n\Psi_0$ . When two of the observables are unbiased (of the type  $X$  and  $P$ ) we always obtained a unique state, regardless of the choice of the third operator: either unbiased or of the type  $X + P$  (biased to the first two), or random. This means that the information provided by two unbiased observables *almost* fixes the state and any other additional information is sufficient to find a unique state. However we know that in the, so called, pathological cases we must find Pauli partners and the algorithm does indeed find them. In these pathological cases, the distributions corresponding to three unbiased operators are all uniform (that is, the generating state  $\Phi$  is unbiased to all three bases). Spanning the Hilbert space by choosing  $\Psi_0$  randomly as a starting state for the algorithm, we converge to all  $N(N - 2) = 3$  Pauli partners with almost equal probability. The pathological case was also studied with two unbiased observables with uniform distributions. In this case the algorithm also delivered all  $N(N - 1) = 6$  Pauli partners with similar probability.

For biased operators, like angular momentum operators  $J_x, J_y, J_z$  and also for random  $A, B, C$  we sometimes found Pauli partners showing that, although we have more equations (six) than unknowns (four), the nonlinearity of the problem may cause non-unique solutions. The appearance of Pauli partners in the angular momentum case is consistent with the result reported by Amiet and Weigert [12]. An inspection of the numerical results for these Pauli partners revealed a symmetry that could also be proved analytically: given a state  $\phi$  (in the basis of  $J_z$ ) with the corresponding distributions for the observables  $J_x, J_y, J_z$ ,

$$\phi = \begin{pmatrix} a \\ b \\ c \end{pmatrix}, \quad (13)$$

(it is always possible to fix  $b$  real and nonnegative) when  $b > 0$  and  $(a^* + c) \neq 0$ , if any one of the following conditions is satisfied:

$$\Re(a) = -\Re(c), \quad (14)$$

$$\Im(a) = \Im(c), \quad (15)$$

$$|a| = |c|, \quad (16)$$

$$\Im(ac) = 0, \quad (17)$$

then there is a Pauli partner  $\phi'$

$$\phi' = \begin{pmatrix} a' \\ b \\ c' \end{pmatrix}, \quad (18)$$

where

$$a' = a^* \frac{(a + c^*)}{(a^* + c)} , \quad c' = c^* \frac{(a^* + c)}{(a + c^*)} . \quad (19)$$

If  $b = 0$  we can make  $a$  real and positive and then  $a' = a$  ,  $c' = c^*$ , and finally if  $(a^* + c) = 0$  then  $c' = -a'^*$ , where  $a'$  can take three values:  $-a$  ,  $ia^*$  ,  $-ia^*$ . Spanning the Hilbert space with generator states  $\phi$  randomly chosen, in some 1% of the cases the algorithm returned the state  $\phi$  and a Pauli partner  $\phi'$  covering all possibilities mentioned above. Notice that the ability of the algorithm to detect Pauli partners is due to the limited precision of the numerical procedure. Among all possible states  $\phi$  of the system, only a few of them have Pauli partners, more precisely, the set of states with Pauli partners has null measure and if we had infinite precision, we would never find partners by random sampling of the Hilbert space. Because of the limited precision of the algorithm, all points in the Hilbert space within a small environment are equivalent and therefore the sets of points with null measure can be accessed in a random sampling of the Hilbert space. We have found indeed that if we become more restrictive with conditions of convergence we need more tries in order to detect partners. Usually the limited precision is considered a drawback however in this case it is an advantage that allows us to detect sets of null measure.

With the information provided by the complete measurement of *four* operators  $A, B, C, D$  we iterated  $\Psi_n = (T_{A\Phi} T_{B\Phi} T_{C\Phi} T_{D\Phi})^n \Psi_0$  and we found unique states, not only when two of them are unbiased (consistent with the result obtained with three operators), but also in the case of random operators or angular momentum in *arbitrary* directions  $J_r, J_s, J_t, J_u$ . Of course, in this case of excessive physical information we could ignore one of the observables and determine the state with only three of them. However not all the Pauli partners found with three observables will have the correct distribution for the fourth one and therefore the use of all observables may be needed for a unique determination of the state. In this case the number of equations, eight if  $N = 3$ , uniquely determine the four unknowns in spite of the nonlinearity. Notice that the convergence of the algorithm in this case is not trivial. It is true that we are using much more information than what is needed (except for the pathological cases that can only appear if  $N > 3$ ) but we must consider that we are using this excessive information in an iterative and approximative algorithm and therefore the consistency of the data in the final state does not necessarily cooperates in the iterations. The fact that the over-determined algorithm converges is a sign of its robustness.

The algorithm converges in a very efficient way, close to exponential, as we see in Figure 3 where the distance to the converging state is given as a function of the number of iterations for the case of three unbiased operators with  $N = 3$ . This is a typical example showing the exponential convergence where the distance to the solution is divided by 4.5 in each iteration. However the speed of convergence, that is, the slope in the figure, is not always the same and depends on the operators used and on the generating state  $\Phi$ . For higher Hilbert space dimensions we obtained similar behaviour. For three operators with physical relevance, like angular momentum or unbiased operators, the distance to the target state was divided by 2-3 in each iteration in Hilbert spaces

with dimensions up to 20. In the fastest case found, the distance was divided by 126 in each iteration, approaching the solution within  $10^{-7}$  after three iterations. With random operators the approach was not always so fast and in some unfavourable cases up to 100 iterations were required (this took only a fraction of a second in an old PC).

## V. CONCLUSION

In this work we defined the *Physical Imposition Operator*  $T_{A\Phi}$  that imposes to any state  $\Psi$  the same distribution that the eigenvalues of an observable  $A$  have in a state  $\Phi$ . For this operator we don't need to know the state  $\Phi$  but we just need the probability distribution for the observable  $A$  in this state, that can be obtained from a complete measurement. Considering two or more observables, we applied their corresponding physical imposition operators iteratively to an arbitrary initial state  $\Psi_0$  and obtained a succession of states  $\Psi_n$  that converge to the unknown state  $\Phi$ , or to a Pauli partner having the same distribution for the observables. Varying the initial state we can find the Pauli partners but we can not be sure that all of them are obtained although this is very likely because in the cases where we can know exactly all the Pauli partners, the algorithm finds them all and therefore it becomes a useful tool for the investigation of Pauli partners. This algorithm for state determination was tested numerically for different sets of observables and different dimensions of the Hilbert space and it turned out to be quite an efficient and robust way to determine a quantum state using complete measurements of several observables.

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## VII. FIGURE CAPTIONS

FIGURE 1. Scatter plot of the distances  $d(\Psi, \Phi)$  and  $d(T_{A\Phi}\Psi, \Phi)$  for 8000 random initial states  $\Psi$ . Points below the diagonal indicate cases where  $T_{A\Phi}$  brings  $\Psi$  closer to  $\Phi$ .

FIGURE 2. Scatter plot of the distances  $d(\Psi, \Phi)$  and  $d(P_{A\Phi}\Psi, \Phi)$  for the same operator and states as in Figure 1. Notice that the Phase Imposition Operator  $P_{A\Phi}$  always approaches the state  $\Phi$ .

FIGURE 3. Distance from the state  $\Psi_n = (T_{A\Phi}T_{B\Phi}T_{C\Phi})^n\Psi_0 = T^n\Psi_0$  to the state  $\Phi$  after  $n$  iterations, showing exponential convergence of the algorithm for  $A, B, C$  unbiased operators in a three dimensional Hilbert space.

This figure "Fig1PhysImpOp.JPG" is available in "JPG" format from:

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